ANALYSIS OF THREE-DIMENSIONAL FRACTURES
SUBJECT TO THERMAL LOADING

by

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June 24, 1991

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ABSTRACT

Formulations have been developed to model three-dimensional fractures in
the presence of thermally-induced strains. Thermal effects are computed
as correction load vectors which are applied to the already existing Surface
Integral and Finite Element Hybrid Method code (SIFEH) for three-
dimensional fracture analysis.

The case of a penny-shaped crack held at constant temperature in an
infinite region has been used to verify the accuracy of the formulations.
Three different mesh densities for the finite element model have been used
to calculate the corresponding stress intensity factors. The calculated
results deviated from the exact solution by 8.93, 0.37, and -0.99% as the
mesh was refined.

Thesis Supervisor: Dr. Michael Cleary

Title: Associate Professor of Mechanical Engineering
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This thesis is dedicated to my parents, Oumayma and Joseph Bsaibes, and to my brothers, Bassam and Shebel Bsaibes, for their continued support, love, and confidence in me.
# Table of Contents

1. **Introduction** ................................................................................................................. 6

2. **Formulation of Governing Matrix Equations**
   2.1 General Overview ........................................................................................................ 8
   2.2 Finite Element Model ................................................................................................. 9
   2.3 Surface Integral Model .............................................................................................. 11
   2.4 Derivation of the \( R^\text{th} \) Vector ....................................................................... 12
   2.5 Derivation of the \( T^\text{th} \) Vector ........................................................................... 15

3. **Results** ...................................................................................................................... 17

4. **Conclusion and Recommendations** ........................................................................... 23

**Appendix A**  
Structure of Frequently Used Matrices ........................................................................... 24

**Appendix B**  
Relationship between Body Stress and Surface Traction ................................................ 27

**Appendix C**  
Listing of Code
   C.1 SUBROUTINE GRTH ................................................................................................. 28
   C.2 SUBROUTINE GTTH ................................................................................................. 50

**Appendix D**  
Flow of Operations in the Code
   D.1 SUBROUTINE GRTH ................................................................................................. 60
   D.2 SUBROUTINE GTTH ................................................................................................. 61

**Appendix E**  
Important Variables in the Code
   E.1 SUBROUTINE GRTH ................................................................................................. 63
   E.2 SUBROUTINE GTTH ................................................................................................. 66

**References** .................................................................................................................... 68
1. Introduction

In this thesis, the capability to account for thermal effects is introduced into the hybrid method developed by Keat [1] for modelling the evolution of three-dimensional cracks in bounded continua. The hybrid method combines the fracture analysis capabilities of the surface integral technique with the finite element method's capacity to incorporate exterior boundary conditions, material inhomogeneities (including nonlinearities), and body forces. The power of this approach lies in the fact that it utilizes the strengths of each of these approaches. For example, the use of the surface integral technique allows effective modelling of the fracture thereby simplifying the discretization process such that a high mesh density near the fracture interface is no longer necessary as would be the case if a finite element model is solely used. Potential applications of the developed capability include its use in modelling the residual stress field at the fiber/matrix interface of a ceramic composite as discussed by Larson [2] and the effect of thermal mismatch between fluid and medium on the growth of underground hydraulic fractures.

This thesis builds on the work of Annigeri [3,4] and Keat [1,4] who developed the Surface Integral and Finite Element Hybrid (SIFEH) method for two- and three-dimensional fracture analysis, respectively. The treatment of volume effects using the hybrid method was first considered by Annigeri [3] who used body force correction vectors to account for far-field plasticity and thermoelastic strains [5] in the two-dimensional hybrid models. Using this work as a basis, this thesis introduces into the three-
dimensional hybrid formulation the capability to model thermoelastic strains.

The remainder of this thesis is divided into three chapters. Chapter 2 presents the formulation of the governing hybrid matrix equations, enhanced to include the effects of thermal strains. Chapter 3 presents results for the case of a penny-shaped crack held at constant temperature in an infinite medium and compares them with the analytical solutions for the stress intensity factor. The last chapter presents conclusions reached and outlines recommendations for further work.
2. Formulation of Governing Matrix Equations

2.1 General Overview

The hybrid formulation used to represent a fracture in a finite medium is based on superposing three separate models. As illustrated in Figure 2.1: Model 1 is a finite element model of the bounded domain with no crack; Model 2 is a surface integral model of the fracture in an infinite region; and finally, Model 3 is another finite element model of the bounded domain with no crack. Correction vectors are needed to ensure that, after superposing the three models, the resultant traction and displacement boundary conditions on the external boundary of the domain as well as on the surface of the fracture remain equivalent to the original situation. Specifically, six correction vectors are computed: \( R^c_2 \), \( R^c_3 \), \( T^th \), \( T^c_1 \), \( T^c_3 \), and \( T^th \). \( R^c_2 \) and \( R^c_3 \) are computed at the location of the external boundary using Models 2 and 3, respectively. These loads are then reversed in sign and applied to Model 1 to satisfy the external traction and displacement boundary conditions. The \( T^th \) vector is a vector of nodal body forces, which when applied to the finite element component of the hybrid model, serves to simulate the thermal strains resulting from the temperature gradient present in the original situation. Similarly, \( T^c_1 \) and \( T^c_3 \) are the tractions occurring in the finite element models on the plane corresponding to the location of the crack. These tractions are reversed in sign and applied to Model 2 in order to satisfy the original traction boundary conditions on the
fracture surface. Note that the $T^\text{th}$ vector is the component of the $T^c_1$ vector that is attributable to the thermal strains.

The governing equations of the hybrid method are derived by coupling the finite element and surface integral model equations as developed by Annigeri [3]. Shorthand matrix notation is used in the derivation below to express those relationships.

**Figure 2.1** Three models are superposed on the right to compose the original problem on the left *(adapted from Keat [1])*.

### 2.2 Finite Element Model

The formulation of the governing matrix equations in the finite element method is well established. Extensive discussions may be found in Cook [6] and Grandin [7]. For the sake of brevity, however, it will suffice to state the governing equation of the finite element model, Model 1, as
\[ [K] \{u^f\} = [R] + [R^{th}] - [R^{c2}] - [R^{c3}] \]  \hspace{1cm} (2.2.1)

where \([K]\) is the finite element stiffness matrix of Model 1; \([u^f]\) is the vector of nodal displacements; \([R]\) is the vector of applied loads, \([R^{th}]\) is a vector of body forces which, when applied to the finite element model, simulates the thermal strains occurring therein; and \([R^{c2}]\) and \([R^{c3}]\) are the correction load vectors. \([R^{c2}]\) is computed using the surface integral formulation as follows:

\[ [R^{c2}] = [G] \{\delta\} \]  \hspace{1cm} (2.2.2)

where \([G]\) is a coupling matrix, and \(\{\delta\}\) represents the crack openings/slip of the fracture surface. On the other hand, \([R^{c3}]\) is expressed using the finite element equations:

\[ [R^{c3}] = [K] \{u^{c3}\} \]  \hspace{1cm} (2.2.3)

where \(\{u^{c3}\}\) in this case is the vector of nodal displacements in Model 3. To enforce displacement boundary conditions on external surfaces, the finite element displacements of Model 3 are required to be equal, but opposite in sign, to the displacements occurring in the surface integral model at those same locations:

\[ \{u^{c3}\} = -\{u^{si}\} = -[L][\delta] \]  \hspace{1cm} (2.2.4)

where \(\{u^{si}\}\) are the surface integral displacements. Combining equations 2.2.3 and 2.2.4, \([R^{c3}]\) may thus be expressed in terms of \(\{\delta\}\) as

\[ [R^{c3}] = -[K][L][\delta] \]  \hspace{1cm} (2.2.5)
Combining equations 2.2.1 - 2.2.5, the governing equation for the finite element model may be expressed in terms of primary variables \( \{u^e\} \) and \( \{\delta\} \) as

\[
[K]\{u^e\} + ([G] - [K][L])\{\delta\} = \{R\} + \{R^{th}\}
\]

2.2.6

### 2.3 Surface Integral Model

The derivation of the surface integral equations modelling the fracture in an infinite region are similarly well established. Using the derivation of Keat [1], the governing relation of Model 2 may be expressed as

\[
[C]\{\delta\} = \{T\} - \{T^{c1}\} - \{T^{c3}\}
\]

2.3.1

where \( \{T\} \) is the known traction boundary condition on the surface of the crack, and \( \{T^{c1}\} \) and \( \{T^{c3}\} \) are the correction vectors associated with Models 1 and 3. \( \{T^{c1}\} \) may be decomposed into

\[
\{T^{c1}\} = \{T^e\} + \{T^{th}\}
\]

2.3.2

where \( \{T^e\} \) is the traction vector resulting from the loads applied to the finite element Model 1 while \( \{T^{th}\} \) is the traction vector resulting from the presence of the temperature gradient. Since \( \{T^e\} \) is evaluated using the finite element equations, we have that:

\[
\{T^e\} = [S]\{u^e\}
\]

2.3.3

Similarly, \( \{T^{c3}\} \) may be expressed in terms of \( \{u^{c3}\} \) as
\[ \{T^c_3\} = [S]\{u^c_3\} \]  \hspace{1cm} 2.3.4

Substitution of equation 2.2.4 into 2.3.4, finally leads to

\[ \{T^c_3\} = -[S][L] \{\delta\} \]  \hspace{1cm} 2.3.5

Combining equations 2.3.1 - 2.3.5, the governing matrix equation for the surface integral model, Model 2, may be expressed in terms of \{u^{fe}\} and \{\delta\} as

\[ [S]\{u^{fe}\} + ([C] - [S][L]) \{\delta\} = \{T\} - \{T^{th}\} \]  \hspace{1cm} 2.3.6

The hybrid equations 2.2.6 and 2.3.6 are coupled via the finite element displacements and the crack openings. These relationships may be written as a pair of simultaneous equations in matrix form as

\[
\begin{bmatrix}
K & G-KL \\
S & C-SL
\end{bmatrix}
\begin{bmatrix}
u^{fe} \\
\delta
\end{bmatrix} =
\begin{bmatrix}
R+R^{th} \\
T-T^{th}
\end{bmatrix}
\]  \hspace{1cm} 2.3.7

2.4 Derivation of the \{R^{th}\} Vector

The \{R^{th}\} vector represents the loading in the finite element model due to the thermal effects. We will derive the composition of this vector by minimizing the total potential energy of the system, \(\Pi\), which is defined by:

\[ \Pi = U + V \]  \hspace{1cm} 2.4.1

where \(U\) is the strain energy and \(V\) is the potential due to the applied loads. We will begin by deriving the strain energy of the system.
The state of stress induced in a single finite element may be expressed as

\[ \{\sigma\} = [C]\{\varepsilon_e\} \quad 2.4.2 \]

where \(\{\sigma\}\), the stress vector, is ordered such that

\[ \{\sigma\} = \{ \sigma_{xx} \ \sigma_{yy} \ \sigma_{zz} \ \sigma_{xy} \ \sigma_{yz} \ \sigma_{xz} \}^T \quad 2.4.3 \]

while \([C]\) is the material matrix, and \(\{\varepsilon_e\}\) is the vector of elastic strains. In the absence of plastic strains, the elastic strain vector can be written as

\[ \{\varepsilon_e\} = \{\varepsilon\} - \{\varepsilon_t\} \quad 2.4.4 \]

where \(\{\varepsilon\}\) is the total strain vector and \(\{\varepsilon_t\}\) is the thermal strain vector as defined below

\[ \{\varepsilon_t\} = \{\alpha \Delta T \ \alpha \Delta T \ \alpha \Delta T \ 0 \ 0 \ 0\} \quad 2.4.5 \]

In equation 2.4.5, \(\alpha\) is the coefficient of thermal expansion and \(\Delta T\) is the imposed temperature change which may vary from point to point within each element in accordance with the shape functions for the three-dimensional brick element.

The strain energy of the element may thus be defined as

\[ U = \frac{1}{2} \iiint [(\varepsilon_e)^T(\sigma)] \, dV \quad 2.4.6 \]

where \(U\) is the strain energy and the integration is done over the volume of the body. Substituting equations 2.4.2 and 2.4.4 into equation 2.4.6, the strain energy may also be expressed by

\[ U = \frac{1}{2} \iiint \left[ (\varepsilon)^T[C](\varepsilon) - (\varepsilon)^T[C](\varepsilon_t) - (\varepsilon_t)^T[C](\varepsilon) + (\varepsilon_t)^T[C](\varepsilon_t) \right] dV \quad 2.4.6a \]
The strain present in a finite element may be related to the nodal displacements using

\[ \{\varepsilon\} = [B]\{u^{fe}\} \]

which upon substitution into equation 2.4.6a leads to the final expression for strain energy:

\[
U = \frac{1}{2} \iiint [\{u^{fe}\}^T[B]^T[C][B]\{u^{fe}\} - \{u^{fe}\}^T[B]^T[C]\{\varepsilon_l\} - \\
-\{\varepsilon_l\}^T[C][B]\{u^{fe}\} + \{\varepsilon_l\}^T[C][\varepsilon_l]\} dV
\]

The potential energy due to the concentrated loads applied at the nodes is expressed by

\[ V = -\{u^{fe}\}^T[R] \]

where \{R\} is the vector of applied loads.

Substituting equations 2.4.6b and 2.4.8 into equation 2.4.1 and minimizing the potential energy with respect to small admissible variations of displacement yields the following result

\[
\frac{\partial P}{\partial \{u^{fe}\}} = 0 = \iiint [B]^T[C][B]dV \{u^{fe}\} - \iiint [B]^T[C][\varepsilon_l]dV - \{R\}
\]

which may be expressed in a simpler form as

\[ 0 = [K]\{u^{fe}\} - \{R^{th}\} - \{R\} \]

where \([K]\) is the stiffness matrix. \(R^{th}\) may thus be explicitly expressed as

\[ \{R^{th}\} = \iint [B]^T[C][\varepsilon_l]dV \]
It should be noted that the above derivation is iterated over the entire assemblage of elements so that the resulting \( R^{th} \) vector represents the global correction vector.

2.5 Derivation of the \( T^{th} \) Vector

The \( T^{th} \) vector representing the traction on the surface of the crack due to the thermal conditions is derived using the finite element equations. Combining equations 2.4.2, 2.4.4, and 2.4.7, stress may be expressed in terms of nodal displacements as

\[
[\sigma] = [C][3][u^{fe}] - [C][\varepsilon]
\]

2.5.1

The traction occurring at a point on the plane of the fracture is defined here in terms of the stress vector

\[
[T^{c_1}] = [\eta][\sigma]
\]

2.5.2

where \([\eta]\), is the matrix composed of the directional cosines defining the orientation of the fracture surface and detailed in Appendix A. Note that \([\sigma]\) is the same stress vector used in the derivation of \( R^{th} \). The use of \([\eta]\) rather than \([n]\) to relate stresses to tractions is done here to accommodate the vector representation of stress as explained in Appendix B. Combining equations 2.5.1 and 2.5.2, the traction correction vector of Model 1 may be expressed as

\[
[T^{c_1}] = [\eta]([C][B][u^{fe}]) - [\eta]([C][\varepsilon])
\]

2.5.3
By comparing equations 2.3.2 and 2.5.3, one would recognize the first term on the right of equation 2.5.3 as \( \{ T^v \} \) and the second term on the right side as \( \{ T^{th} \} \). That is, \( \{ T^{th} \} \) may be computed as

\[
\{ T^{th} \} = -[\eta][C][\varepsilon_1]
\]

This \( \{ T^{th} \} \) is represented in global coordinates. In order to represent it in coordinates local to the fracture surface, a transformation matrix, \( [Q] \), composed of the directional cosines of the surface and detailed in Appendix A, is used such that

\[
\{ T^{th} \} = -[Q][\eta][C][\varepsilon_1]
\]

\( \{ T^{th} \} \) is calculated in this manner at all points on the fracture surface and assembled in the corresponding global traction correction vector.
3. Results

Two subroutines, GRTH and GTTH listed in Appendix C, were written in Fortran to calculate the \( R^{th} \) and \( T^{th} \) correction vectors of equations 2.4.11 and 2.5.5. Appendix D contains a brief description of the flow of operations in GRTH and GTTH. These subroutines were embedded into the SIFEH code developed by Keat [1].

The accuracy of the \( R^{th} \) and \( T^{th} \) calculations was tested for the case of a penny-shaped crack at uniform constant temperature in an infinite region. The analytical solution for the temperature field is stated by Carslaw and Jaeger [8] as

\[
T = \frac{2T_0}{\pi} \sin^{-1}\left(\frac{2a}{\sqrt{(r-a)^2 + z^2} + \sqrt{(r+a)^2 + z^2}}\right)
\]

for \( z > 0 \) \hspace{1cm} 3.1

\[
T = \frac{2T_0}{\pi} \sin^{-1}\left(\frac{\bar{a}}{r}\right)
\]

\( r > a, \ z = 0 \) \hspace{1cm} 3.2

\[
T = T_0
\]

\( r \leq a, \ z = 0 \) \hspace{1cm} 3.3

where \( T \) is the temperature sought, \( z \) is the perpendicular distance from the plane of the crack, \( r \) is the radial distance from the center of the crack, \( T_0 \) is the fixed temperature of the fracture, and \( a \) is the radius of the crack.

Figure 3.1 on the following page illustrates the temperature distribution given by equations 3.1-3.3.
Figure 3.1 (a) Distribution of the temperature field as a function of (a) radial distance, $r$, and (b) perpendicular distance, $z$, from the crack surface. Note that $a=1.0$ and $T_0=100$ for this crack.

The exact stress intensity factor, $K_I$, for this geometry and thermal conditions, may be obtained from Murakami [9] as

$$K_I = \left( \frac{E \alpha}{\sqrt{\pi} (1-\nu)} \right) T_0 \sqrt{a}$$

where $E$ and $\nu$ are the Young's modulus and Poisson's ratio respectively, $T_0$ is the temperature of the crack, and $\alpha$ is the coefficient of thermal expansion. It is evident from Figure 3.1 that the temperature changes dramatically in the vicinity of the crack tip ($r = a = 1.0$).
The finite element meshes of Figure 3.2 were used to discretize the infinite medium without the crack. This mesh was rotated about an axis of symmetry, the z-axis, to create a volume of revolution with one-eighth symmetry (the plane of the fracture is also a plane of symmetry). The density of the mesh in the rotational direction about the axis of symmetry was also varied as illustrated by Figure 3.3. It should be noted that the elements of the meshes of Figures 3.2 and 3.3 are intentionally made smaller in size close to the crack tip \( r = a = 1.0 \) so as to capture as accurately as possible the steep temperature gradients of Figures 3.1. The crack mesh used to discretize the fracture in the surface integral model is illustrated in Figure 3.4. The interpolation functions used to represent the crack opening are linear in the interior of the fracture and assume a \( p^{1/2} \) variation of crack opening in the elements along the fracture perimeter, where \( p \) is the perpendicular distance from the crack front.

The stress intensity factors computed using the different mesh densities and the associated numerical errors are recorded in Table 3.1. Mesh 1 is composed of the meshes illustrated in Figures 3.2a and 3.3a. Mesh 2 is composed of the meshes illustrated in Figures 3.2c and 3.3a, while mesh 3 is composed of the meshes of Figures 3.2c and 3.3b. One may note that high accuracies in \( K_I \) were obtained using relatively coarse finite element meshes. It is also interesting to note that the error between the calculated stress intensity factors and the analytical value is positive for meshes 1 and 2 while it is negative for mesh 3. The change in sign is due to the interaction of the errors in the finite element and the surface integral formulations. The finite element method generally tends to decrease in
stiffness as the number of nodes is increased as opposed to the surface integral method which increases in stiffness.

Figure 3.2  Meshes used to discretize the infinite medium. (a) Overview of the coarse mesh  (b) Magnified view of the coarse mesh. (c) Overview of the fine mesh.  (d) Magnified view of the fine mesh. Note that a=1.0 for this crack.
Figure 3.3  Top view of the model showing the mesh densities in the rotational direction. (a) Coarse mesh with three elements in the rotational direction. (b) Finer mesh with five elements in the rotational direction.
Figure 3.4  The mesh used to discretize the crack in the surface integral model. (*Courtesy of Keat [1]*)

Table 3.1  Comparison of the exact solution with results obtained by the different mesh densities (*E*=6x10^6, *v*=0.3, *α*=0.5, *T_0*=10.0, *a*=1.0).

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Nodes</th>
<th>Elements</th>
<th>( K_i^{calc}(10^6) )</th>
<th>( K_i^{exact}(10^6) )</th>
<th>Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>196</td>
<td>108</td>
<td>-26.34</td>
<td>-24.18</td>
<td>8.93</td>
</tr>
<tr>
<td>2</td>
<td>256</td>
<td>147</td>
<td>-24.27</td>
<td>-24.18</td>
<td>0.37</td>
</tr>
<tr>
<td>3</td>
<td>384</td>
<td>245</td>
<td>-23.94</td>
<td>-24.18</td>
<td>-0.99</td>
</tr>
</tbody>
</table>
4. Conclusion and Recommendations

Formulations for calculating three-dimensional thermally induced strains using the Surface Integral and Finite Element Hybrid method have proven to be very accurate. The test case of a penny-shaped crack held at constant temperature in an infinite medium produced results that were very close to the exact solutions despite the relative coarseness of the finite element meshes used. Errors in $K_I$ of 8.93, 0.37, and -0.99\% resulted as the finite element mesh was progressively refined, while holding the surface integral mesh constant.

The development of these formulations and the code to calculate the correction vectors open new horizons for further work. Though only one geometry has been examined here, the current capability can also be used to model such problems as tilted cracks and media with position-dependent material properties. Problems containing cracks with uniform heat flow can also be modelled provided that the temperature distribution field in the medium is known or can be calculated using heat transfer finite element analysis.
Appendix A  Structure of Frequently Used Matrices

This appendix details the structure of the matrices appearing in the hybrid formulations. These include: $\{\epsilon\}$, $\{\epsilon_t\}$, $\{\sigma\}$, $[C]$, $[B]$, $[R]$, $[Q]$, and $[\eta]$. 

$$\{\epsilon\} = [\epsilon_{xx} \epsilon_{yy} \epsilon_{zz} \epsilon_{xy} \epsilon_{yz} \epsilon_{xz}]^T$$

$$\{\epsilon_t\} = [\alpha \Delta T \alpha \Delta T \alpha \Delta T 0 0 0]^T$$

where $\alpha$ is the coefficient of thermal expansion and $\Delta T$ is the imposed change in temperature.

$$\{\sigma\} = [\sigma_{xx} \sigma_{yy} \sigma_{zz} \sigma_{xy} \sigma_{yz} \sigma_{xz}]^T$$

$$[C] = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1 & A & A & 0 & 0 & 0 \\ A & 1 & A & 0 & 0 & 0 \\ A & A & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & B & 0 & 0 \\ 0 & 0 & 0 & 0 & B & 0 \\ 0 & 0 & 0 & 0 & 0 & B \end{bmatrix}$$

where

$$A = \frac{\nu}{1-\nu} \quad B = \frac{1-2\nu}{2(1-\nu)}$$

where $E$ and $\nu$ are the Young's modulus and Poisson's ratio, respectively.
The strain-displacement matrix, \([B]\), is defined in accordance with the definition of \(\{\varepsilon\}\)

\[
[B] = \begin{bmatrix}
H_{1x} & 0 & 0 & H_{1y} & 0 & H_{1z} \\
0 & H_{1y} & 0 & H_{1x} & H_{1z} & 0 \\
0 & 0 & H_{1z} & 0 & H_{1y} & H_{1x} \\
H_{2x} & 0 & 0 & H_{2y} & 0 & H_{2z} \\
0 & H_{2y} & 0 & H_{2x} & H_{2z} & 0 \\
0 & 0 & H_{2z} & 0 & H_{2y} & H_{2x} \\
H_{3x} & 0 & 0 & H_{3y} & 0 & H_{3z} \\
0 & H_{3y} & 0 & H_{3x} & H_{3z} & 0 \\
0 & 0 & H_{3z} & 0 & H_{3y} & H_{3x} \\
H_{4x} & 0 & 0 & H_{4y} & 0 & H_{4z} \\
0 & H_{4y} & 0 & H_{4x} & H_{4z} & 0 \\
0 & 0 & H_{4z} & 0 & H_{4y} & H_{4x} \\
H_{5x} & 0 & 0 & H_{5y} & 0 & H_{5z} \\
0 & H_{5y} & 0 & H_{5x} & H_{5z} & 0 \\
0 & 0 & H_{5z} & 0 & H_{5y} & H_{5x} \\
H_{6x} & 0 & 0 & H_{6y} & 0 & H_{6z} \\
0 & H_{6y} & 0 & H_{6x} & H_{6z} & 0 \\
0 & 0 & H_{6z} & 0 & H_{6y} & H_{6x} \\
H_{7x} & 0 & 0 & H_{7y} & 0 & H_{7z} \\
0 & H_{7y} & 0 & H_{7x} & H_{7z} & 0 \\
0 & 0 & H_{7z} & 0 & H_{7y} & H_{7x} \\
H_{8x} & 0 & 0 & H_{8y} & 0 & H_{8z} \\
0 & H_{8y} & 0 & H_{8x} & H_{8z} & 0 \\
0 & 0 & H_{8z} & 0 & H_{8y} & H_{8x}
\end{bmatrix}
\]

where

\[
H_{nx} = \frac{\partial h_n}{\partial x} \quad H_{ny} = \frac{\partial h_n}{\partial y} \quad H_{nz} = \frac{\partial h_n}{\partial z}
\]
where $h_n$ is the $n$th corresponding shape, or interpolation, function for an isoparametric eight-noded cube element.

$$[R] = [R_{1x} \ R_{1y} \ R_{1z} \ R_{2x} \ R_{2y} \ R_{2z} \ R_{3x} \ R_{3y} \ R_{3z} \ .......]^T$$

where $R_{nx}$, $R_{ny}$, and $R_{nz}$ are the respective components of the nodal forces acting on node $n$ in the $x$, $y$, and $z$ directions respectively.

$$[Q] = \begin{bmatrix} t_x & t_y & t_z \\ s_x & s_y & s_z \\ n_x & n_y & n_z \end{bmatrix}$$

where $t$ and $s$ are orthogonal vectors defined in the plane of the crack, and $n$ is perpendicular to the crack. The subscripts $x$, $y$, and $z$ represent the components of each directional vector in the global $x$, $y$, and $z$ directions respectively. $[\eta]$ is also defined with this notation as

$$[\eta] = \begin{bmatrix} n_x & 0 & 0 & n_y & 0 & n_z & 0 & n_y & n_x \end{bmatrix}$$
Appendix B  Relationship Between Body Stress and Surface Traction

Traditionally, the relationship between surface tractions and stresses is expressed as

\[ \{t\} = [\sigma][n] \]

where \( \{t\} \) is the vector of tractions, \([\sigma]\) is the stress tensor of the form

\[ [\sigma] = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix} \]

and the normal vector \( \{n\} \), expressed in terms of its global components,

\[ \{n\} = \{n_x \ n_y \ n_z\}^T \]

defines the plane on which the traction is present.

The same relationship may be equivalently stated by writing stress as a vector, which is a more conventional representation when using finite elements,

\[ \{T\} = [\eta][\sigma] \]

where the structures of \([\eta]\) and \(\{\sigma\}\) are detailed in Appendix A.
where $h_n$ is the $n$th corresponding shape, or interpolation, function for an isoparametric eight-noded cube element.

$$\{R\} = \{R_{1x} \ R_{1y} \ R_{1z} \ R_{2x} \ R_{2y} \ R_{2z} \ R_{3x} \ R_{3y} \ R_{3z} \ \ldots\ldots\}^T$$

where $R_{nx}$, $R_{ny}$, and $R_{nz}$ are the respective components of the nodal forces acting on node $n$ in the x, y, and z directions respectively.

$$[Q] = \begin{bmatrix} t_x & t_y & t_z \\ s_x & s_y & s_z \\ n_x & n_y & n_z \end{bmatrix}$$

where $t$ and $s$ are orthogonal vectors defined in the plane of the crack, and $n$ is perpendicular to the crack. The subscripts $x$, $y$, and $z$ represent the components of each directional vector in the global $x$, $y$, and $z$ directions respectively. $[\eta]$ is also defined with this notation as

$$[\eta] = \begin{bmatrix} n_x & 0 & 0 & n_y & 0 & n_z \\ 0 & n_y & 0 & n_x & n_z & 0 \\ 0 & 0 & n_z & 0 & n_y & n_x \end{bmatrix}$$
Appendix B  Relationship Between Body Stress and Surface Traction

Traditionally, the relationship between surface tractions and stresses is expressed as

\[
\{t\} = [\sigma]\{n\}
\]

where \(\{t\}\) is the vector of tractions, \([\sigma]\) is the stress tensor of the form

\[
[\sigma] = \begin{bmatrix}
\sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\
\sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\
\sigma_{zx} & \sigma_{zy} & \sigma_{zz}
\end{bmatrix}
\]

and the normal vector \(\{n\}\), expressed in terms of its global components,

\[
\{n\} = [n_x \ n_y \ n_z]^T
\]

defines the plane on which the traction is present.

The same relationship may be equivalently stated by writing stress as a vector, which is a more conventional representation when using finite elements,

\[
\{T\} = [\eta][\sigma]
\]

where the structures of \([\eta]\) and \([\sigma]\) are detailed in Appendix A.
Appendix C  Listing of Code

C.1 SUBROUTINE GRTH

C *********************************************************************************************
SUBROUTINE GRTH(COR, NUME, NOD, E, V, ALPHA, TEMPNI, TEMPNF, RTH)

C *********************************************************************************************

DIMENSION COR(100, 1), NOD(10, 1), RTH(1), E(1), V(1), ALPHA(1)
DIMENSION TEMPNI(10, 1), TEMPNF(10, 1)
DIMENSION D(3, 3), DH(3, 8), DDH(3, 8), B(6, 24), BB(24, 6), C(6, 6)
DIMENSION ETHERM(6), TMP(24, 6), PRD(24), LRTH(24)
DIMENSION X(8), Y(8), Z(8), R(3), S(3), T(3), W(3), TX(3)

INTEGER II, JJ, KK, GORDER, LORDER, ELT
REAL PRD, LRTH

C
C INITIALIZE VARIABLES THAT ARE NOT READ OR DIRECTLY ASSIGNED
C

DO 10 I = 1, 3

28
DO 5 J=1, 3
    D(I,J) = 0
5    CONTINUE
DO 8 J=1, 8
    DH(I,J) = 0
8    CONTINUE
10   CONTINUE

CALL GAUSS(R,S,T,W,INTPT)

C       PERFORM THE GAUSSIAN INTEGRATION (SUMMATION)
C       OVER THE GAUSSIAN POINTS
DO 510 ELT=1, NUME
    DO 32 I=1,24
        LRTH(I) = 0.0
32   CONTINUE
DO 500 II=1, INTPT
    DO 490 JJ=1, INTPT
        DO 480 KK=1, INTPT
            CALL INIT(DDH,PRD,TMP,B,BB)
            CALL COORD(COR,NOD,ELT,X,Y,Z)
            CALL DIFF(X,Y,Z,R,S,T,II,JJ,KK,DXDR,DXDS,DXDT,
              DYDR, DYDS, DYDT, DZDR, DZDS, DZDT)
            CALL DMRX(DXDR,DXDS,DXDT,DYDR,DYDS,DYDT,
              DZDR,DZDS,DZDT,DET,D)
            CALL DHMRX(R,S,T,II,JJ,KK,DH)
        CALL DDHMRX(D,DH,DDH)
CALL BMRX(DDH,B)
CALL BTRANS(B,BB)
TX(1) = R(II)
TX(2) = S(JJ)
TX(3) = T(KK)
TEMP = TEMPER(TEMPNI,TEMPNF,ELT,TX)
CALL STRAIN(ALPHA(ELT),TEMP,ETHERM)
CALL MTRL(E(ELT),V(ELT),C)
CALL LOCAL(TMP,BB,C,PRD,ETHERM,W,DET,II,
1
JJ,KK,LRTH)
480 CONTINUE
490 CONTINUE
500 CONTINUE
DO 505 I=1, 8
   GORDER = (NOD(ELT,I)-1)*3
   LORDER = (I-1)*3
DO 507 J=1,3
   RTH(GORDER+J) = RTH(GORDER+J) + LRTH(LORDER+J)
507 CONTINUE
505 CONTINUE
510 CONTINUE
RETURN
END
**C******************************************************************************

SUBROUTINE GAUSS(R,S,T,W,INTPT)

**C******************************************************************************

DIMENSION R(1), S(1), T(1), W(1)

**C SET 2-POINT GAUSS QUADRATURE INTEGRATION POINTS AND WEIGHTS**

INTPT = 2
R(1) = -0.5773503
R(2) =  0.5773503
R(3) =  0.00
S(1) = -0.5773503
S(2) =  0.5773503
S(3) =  0.00
T(1) = -0.5773503
T(2) =  0.5773503
T(3) =  0.00
W(1) = 1.0
W(2) = 1.0
W(3) = 0.0

END
SUBROUTINE MTRL(E,V,C)

DIMENSION C(6,1)

C FILLING UP THE C MATRIX (MATERIAL MATRIX)

\[ REL = \frac{E(1-V)}{(1+V)(1-2V)} \]

\[ C(1,1) = REL \]
\[ C(1,2) = RELV/(1-V) \]
\[ C(1,3) = RELV/(1-V) \]
\[ C(1,4) = 0 \]
\[ C(1,5) = 0 \]
\[ C(1,6) = 0 \]
\[ C(2,1) = RELV/(1-V) \]
\[ C(2,2) = REL \]
\[ C(2,3) = RELV/(1-V) \]
\[ C(2,4) = 0 \]
\[ C(2,5) = 0 \]
\[ C(2,6) = 0 \]
\[ C(3,1) = RELV/(1-V) \]
\[ C(3,2) = RELV/(1-V) \]
\[ C(3,3) = REL \]
\[ C(3,4) = 0 \]
C(3,5) = 0
C(3,6) = 0
C(4,1) = 0
C(4,2) = 0
C(4,3) = 0
C(4,4) = REL*(1-2*V)/( 2*(1-V) )
C(4,5) = 0
C(4,6) = 0
C(5,1) = 0
C(5,2) = 0
C(5,3) = 0
C(5,4) = 0
C(5,5) = REL*(1-2*V)/( 2*(1-V) )
C(5,6) = 0
C(6,1) = 0
C(6,2) = 0
C(6,3) = 0
C(6,4) = 0
C(6,5) = 0
C(6,6) = REL*(1-2*V)/( 2*(1-V) )
END
SUBROUTINE STRAIN(ALPHA,TEMP,ETHERM)

DIMENSION ETHERM(1)

COMPOSE THE ETHERM MATRIX (THERMAL STRAIN MATRIX)

DO 700 I=1,6
   IF (I .LE. 3) THEN
      ETHERM(I) = ALPHA*TEMP
   ELSE
      ETHERM(I) = 0.
   END IF
700   CONTINUE

END

SUBROUTINE INIT(ΩDH,PRD,TMP,B,BB)
DIMENSION DDH(3,1), PRD(1), TMP(24,1), B(6,1), BB(24,1)

DO 85 I=1, 3
   DO 80 J=1, 8
      DDH(I,J) = 0.0
   CONTINUE
   CONTINUE

DO 87 I=1, 24
   PRD(I) = 0.0
   DO 81 J=1, 6
      TMP(I,J)=0.0
      B(J,I) = 0.0
      BB(I,J) = 0.0
   CONTINUE
   CONTINUE

END

C *******************************************************
SUBROUTINE COORD(COR,NOD,ELT,X,Y,Z)
C *******************************************************
DIMENSION COR(100,1), NOD(10,1), X(1), Y(1), Z(1)

INTEGER ELT

C ASSIGN THE COORDINATES OF THE NODES OF THE
C ELEMENT AT HAND TO VALUES OF X(I),Y(I),Z(I)

DO 90 I=1, 8
   X(I) = COR(NOD(ELT,I),1)
   Y(I) = COR(NOD(ELT,I),2)
   Z(I) = COR(NOD(ELT,I),3)
90 CONTINUE
END

C ***********************************************
1 DXDT,DYDR,DYDS,DYDT,DZDR,DZDS,DZDT)
C ***********************************************

DIMENSION X(1),Y(1),Z(1),R(1),S(1),T(1)

DXDR = (1/8)*((1+S(JJ))*(1+T(KK)))*X(1) +
\((-1-S(JJ))*(1+T(KK))*X(2) +
\)  
\((-1+S(JJ))*(1+T(KK))*X(3) +
\)  
\((1-S(JJ))*(1+T(KK))*X(4) +
\)  
\((1+S(JJ))*(1-T(KK))*X(5) +
\)  
\((-1-S(JJ))*(1-T(KK))*X(6) +
\)  
\((-1+S(JJ))*(1-T(KK))*X(7) +
\)  
\((1-S(JJ))*(1-T(KK))*X(8))

\[\text{DXDS} = (1/8)*((1+R(II))*(1+T(KK))*X(1) +
\]  
\((1-R(II))*(1+T(KK))*X(2) +
\)  
\((-1+R(II))*(1+T(KK))*X(3) +
\)  
\((-1-R(II))*(1+T(KK))*X(4) +
\)  
\((1+R(II))*(1-T(KK))*X(5) +
\)  
\((1-R(II))*(1-T(KK))*X(6) +
\)  
\((-1+R(II))*(1-T(KK))*X(7) +
\)  
\((-1-R(II))*(1-T(KK))*X(8))\]

\[\text{DXDT} = (1/8)*((1+S(JJ)+R(II)+R(II)*S(JJ))*X(1) +
\]  
\((1+S(JJ)-R(II)-R(II)*S(JJ))*X(2) +
\)  
\((1-S(JJ)-R(II)+R(II)*S(JJ))*X(3) +
\)  
\((1-S(JJ)+R(II)-R(II)*S(JJ))*X(4) +
\)  
\((-1-S(JJ)-R(II)-R(II)*S(JJ))*X(5) +
\)  
\((-1+S(JJ)+R(II)+R(II)*S(JJ))*X(6) +
\)  
\((-1+S(JJ)+R(II)-R(II)*S(JJ))*X(7) +
\)  
\((-1+S(JJ)-R(II)+R(II)*S(JJ))*X(8))\]
DYDR = (1/8)*((1+S(JJ))*(1+T(KK))*Y(1) +
1 (-1-S(JJ))*(1+T(KK))*Y(2) +
2 (-1+S(JJ))*(1+T(KK))*Y(3) +
3 (1-S(JJ))*(1+T(KK))*Y(4) +
4 (1+S(JJ))*(1-T(KK))*Y(5) +
5 (-1-S(JJ))*(1-T(KK))*Y(6) +
6 (-1+S(JJ))*(1-T(KK))*Y(7) +
7 (1-S(JJ))*(1-T(KK))*Y(8))

DYDS = (1/8)*((1+R(II))*(1+T(KK))*Y(1) +
1 (1-R(II))*(1+T(KK))*Y(2) +
2 (-1+R(II))*(1+T(KK))*Y(3) +
3 (-1-R(II))*(1+T(KK))*Y(4) +
4 (1+R(II))*(1-T(KK))*Y(5) +
5 (1-R(II))*(1-T(KK))*Y(6) +
6 (-1+R(II))*(1-T(KK))*Y(7) +
7 (-1-R(II))*(1-T(KK))*Y(8))

DYDT = (1/8)*((1+S(JJ)+R(II)+R(II)*S(JJ))*Y(1) +
1 (1+S(JJ)-R(II)-R(II)*S(JJ))*Y(2) +
2 (1-S(JJ)-R(II)+R(II)*S(JJ))*Y(3) +
3 (1-S(JJ)+R(II)-R(II)*S(JJ))*Y(4) +
4 (-1-S(JJ)-R(II)-R(II)*S(JJ))*Y(5) +
5 (-1-S(JJ)+R(II)+R(II)*S(JJ))*Y(6) +
6 (-1+S(JJ)+R(II)-R(II)*S(JJ))*Y(7) +
7 (-1+S(JJ)-R(II)+R(II)*S(JJ))*Y(8))
\[ DZDR = (1/8)\times((1+S(JJ))\times(1+T(KK))\times Z(1) + \\
\times (-1-S(JJ))\times(1+T(KK))\times Z(2) + \\
\times (-1+S(JJ))\times(1+T(KK))\times Z(3) + \\
\times (1-S(JJ))\times(1+T(KK))\times Z(4) + \\
\times (1+S(JJ))\times(1-T(KK))\times Z(5) + \\
\times (-1-S(JJ))\times(1-T(KK))\times Z(6) + \\
\times (-1+S(JJ))\times(1-T(KK))\times Z(7) + \\
\times (1-S(JJ))\times(1-T(KK))\times Z(8)) \]

\[ DZDS = (1/8)\times((1+R(II))\times(1+T(KK))\times Z(1) + \\
\times (1-R(II))\times(1+T(KK))\times Z(2) + \\
\times (-1+R(II))\times(1+T(KK))\times Z(3) + \\
\times (-1-R(II))\times(1+T(KK))\times Z(4) + \\
\times (1+R(II))\times(1-T(KK))\times Z(5) + \\
\times (1-R(II))\times(1-T(KK))\times Z(6) + \\
\times (-1+R(II))\times(1-T(KK))\times Z(7) + \\
\times (-1-R(II))\times(1-T(KK))\times Z(8)) \]

\[ DZDT = (1/8)\times((1+S(JJ)+R(II)+R(II)\times S(JJ))\times Z(1) + \\
\times (1+S(JJ)-R(II)-R(II)\times S(JJ))\times Z(2) + \\
\times (1-S(JJ)-R(II)+R(II)\times S(JJ))\times Z(3) + \\
\times (1-S(JJ)+R(II)-R(II)\times S(JJ))\times Z(4) + \\
\times (-1-S(JJ)-R(II)-R(II)\times S(JJ))\times Z(5) + \\
\times (-1-S(JJ)+R(II)+R(II)\times S(JJ))\times Z(6) + \\
\times (-1+S(JJ)+R(II)-R(II)\times S(JJ))\times Z(7) + \\
\times (-1+S(JJ)+R(II)-R(II)\times S(JJ))\times Z(8)) \]
(-1+S(JJ)-R(II)+R(II)*S(JJ))*Z(8))

END

C *********************************************************************************************************************
SUBROUTINE DMRX(DXDR,DXDS,DXDT,DYDR,DYDS,DYDT,
1 DZDR,DZDS,DZDT,DET,D)
C *********************************************************************************************************************

DIMENSION D(3,1)

C DEFINE THE D MATRIX (THE INVERSE OF THE JACOBIAN C MATRIX) (ASSUMED THAT MATRIX INVERSE DOES NOT C INVOLVE MULTIPLYING ORIGINAL ELEMENTS WITH C COFACTOR MATRIX. NEED TO CHECK. 2/5/91)

DET = DXDR*((DYDS*DZDT)-(DZDS*DYDT)) -
1 DYDR*((DXDS*DZDT)-(DZDS*DXDT)) +
2 DZDR*((DXDS*DYDT)-(DYDS*DXDT))

D(1,1) = (1/DET)*((DYDS*DZDT)-(DZDS*DYDT))
D(1,2) = (1/DET)*(-1)*((DYDR*DZDT)-(DZDR*DYDT))
D(1,3) = (1/DET)*((DYDR*DZDS)-(DZDR*DYDS))
D(2,1) = (1/DET)*(-1)*((DXDS*DZDT)-(DZDS*DXDT))
\[ D(2,2) = \frac{1}{DET} \times ((DXDR*DXDT) - (DZDR*DXDT)) \]
\[ D(2,3) = \frac{1}{DET} \times (-1) \times ((DXDR*DYDT) - (DZDR*DXDS)) \]
\[ D(3,1) = \frac{1}{DET} \times ((DXDS*DYDT) - (DYDS*DXDT)) \]
\[ D(3,2) = \frac{1}{DET} \times (-1) \times ((DXDR*DYDT) - (DYDR*DXDT)) \]
\[ D(3,3) = \frac{1}{DET} \times ((DXDR*DYDS) - (DYDR*DXDS)) \]

END

C

******************************************************************************

SUBROUTINE DHMRX(R,S,T,II,JJ,KK,DH)

******************************************************************************

DIMENSION DH(3,1), R(1), S(1), T(1)

C

DEFINE THE DH MATRIX

C

\[ DH(1,1) = (1/8) \times (1+S(JJ)) \times (1+T(KK)) \]
\[ DH(2,1) = (1/8) \times (1+R(II)) \times (1+T(KK)) \]
\[ DH(3,1) = (1/8) \times (1+S(JJ)+R(II)+R(II) \times S(JJ)) \]
\[ DH(1,2) = (1/8) \times (-1-S(JJ)) \times (1+T(KK)) \]
\[ DH(2,2) = (1/8) \times (1-R(II)) \times (1+T(KK)) \]
\[ DH(3,2) = (1/8)\star (1 + S(JJ) - R(II) - R(II) \star S(JJ)) \]

\[ DH(1,3) = (1/8)\star (-1 + S(JJ)) \star (1 + T(KK)) \]
\[ DH(2,3) = (1/8)\star (-1 + R(II)) \star (1 + T(KK)) \]
\[ DH(3,3) = (1/8)\star (1 - S(JJ) - R(II) + R(II) \star S(JJ)) \]

\[ DH(1,4) = (1/8)\star (1 - S(JJ)) \star (1 + T(KK)) \]
\[ DH(2,4) = (1/8)\star (-1 - R(II)) \star (1 + T(KK)) \]
\[ DH(3,4) = (1/8)\star (1 - S(JJ) + R(II) - R(II) \star S(JJ)) \]

\[ DH(1,5) = (1/8)\star (1 + S(JJ)) \star (1 - T(KK)) \]
\[ DH(2,5) = (1/8)\star (1 + R(II)) \star (1 - T(KK)) \]
\[ DH(3,5) = (1/8)\star (-1 - S(JJ) - R(II) - R(II) \star S(JJ)) \]

\[ DH(1,6) = (1/8)\star (-1 - S(JJ)) \star (1 - T(KK)) \]
\[ DH(2,6) = (1/8)\star (1 - R(II)) \star (1 - T(KK)) \]
\[ DH(3,6) = (1/8)\star (-1 - S(JJ) + R(II) + R(II) \star S(JJ)) \]

\[ DH(1,7) = (1/8)\star (-1 + S(JJ)) \star (1 - T(KK)) \]
\[ DH(2,7) = (1/8)\star (-1 + R(II)) \star (1 - T(KK)) \]
\[ DH(3,7) = (1/8)\star (-1 + S(JJ) + R(II) - R(II) \star S(JJ)) \]

\[ DH(1,8) = (1/8)\star (1 - S(JJ)) \star (1 - T(KK)) \]
\[ DH(2,8) = (1/8)\star (-1 - R(II)) \star (1 - T(KK)) \]
\[ DH(3,8) = (1/8)\star (-1 + S(JJ) - R(II) + R(II) \star S(JJ)) \]
SUBROUTINE DDHMRX(D,DH,DI,H)

DIMENSION D(3,1), DH(3,1), DDH(3,1)

COMPOSE THE DDH MATRIX FROM THE D MATRIX AND THE DH MATRIX

DO 120 I=1,8
   DO 110 J=1,3
      DO 100 K=1,3
         DDH(J,I) = DDH(J,I) + D(J,K)*DH(K,I)
      100 CONTINUE
   110 CONTINUE
120 CONTINUE

END
SUBROUTINE BMRX(DDH,B)

DIMENSION DDH(3,1), B(6,1)

INTEGER FLAG

C FILL UP THE B MATRIX

DO 190 I=1,6
   FLAG = 0
   IF (I .EQ. 1) THEN
      DO 130 J=1,22,3
         FLAG = FLAG + 1
         B(I,J) = DDH(1,FLAG)
         B(I,J+1) = 0
         B(I,J+2) = 0
      CONTINUE
   ELSE IF (I .EQ. 2) THEN
      DO 140 J=1,22,3
         FLAG = FLAG + 1
         B(I,J) = 0
         B(I,J+1) = DDH(2,FLAG)
         B(I,J+2) = 0
      CONTINUE
   END IF

190 CONTINUE
ELSE IF (I .EQ. 3) THEN
  DO 150 J=1,22,3
    FLAG = FLAG + 1
    B(I,J) = 0
    B(I,J+1) = 0
    B(I,J+2) = DDH(3,FLAG)
  150 CONTINUE

ELSE IF (I .EQ. 4) THEN
  DO 160 J=1,22,3
    FLAG = FLAG + 1
    B(I,J) = DDH(2,FLAG)
    B(I,J+1) = DDH(1,FLAG)
    B(I,J+2) = 0
  160 CONTINUE

ELSE IF (I .EQ. 5) THEN
  DO 170 J=1,22,3
    FLAG = FLAG + 1
    B(I,J) = 0
    B(I,J+1) = DDH(3,FLAG)
    B(I,J+2) = DDH(2,FLAG)
  170 CONTINUE

ELSE
  DO 180 J=1,22,3
    FLAG = FLAG + 1
    B(I,J) = DDH(3,FLAG)
    B(I,J+1) = 0
  180 CONTINUE

B(I,J+2) = DDH(1,FLAG)

180 CONTINUE

END IF

190 CONTINUE

END

C ******************************************************************************

SUBROUTINE BTRANS(B,BB)

C ******************************************************************************

DIMENSION B(6,1), BB(24,1)

C  TRANSPOSE THE B MATRIX

      DO 210 I=1,6

          DO 200 J=I,24

              BB(J,I) = B(I,J)

      200 CONTINUE

210 CONTINUE

END
SUBROUTINE LOCAL(TMP, BB, C, P, E, W, DET, II, JJ,  
1    KK, LRTH)

DIMENSION TMP(24,1), BB(24,1), C(6,1), P(1), E(1), W(1)
DIMENSION LRTH(1)

REAL LRTH

C   MULTPLY B-TRNSPOSE MATRIX, C MATRIX, AND  
C   ETHERM MATRIX

DO 740 I=1,6
  DO 730 J=1,24
    DO 725 K=1,6
      TMP(J,I) = TMP(J,I) + BB(J,K)*C(K,I)
    725    CONTINUE
  730    CONTINUE
  740    CONTINUE

DO 760 I=1,24
  DO 755 J=1,6
    PRD(I) = PRD(I) + TMP(I,J)*E(J)
  755    CONTINUE
  760    CONTINUE
\text{WEIGHT} = W(II) \times W(JJ) \times W(KK)

\text{DO 300 I=1, 24}

\hspace{1cm} \text{PRD(I) = PRD(I) \times DET}

\hspace{1cm} \text{PRD(I) = PRD(I) \times WEIGHT}

\text{300 CONTINUE}

\text{DO 743 I=1, 24}

\hspace{1cm} \text{LRTH(I) = LRTH(I) + PRD(I)}

743 \hspace{0.5cm} \text{CONTINUE}

\text{END}

\text{C} \hspace{1cm} \text{*******************************************************}

\text{FUNCTION TEMPER(TEMPNI,TEMPNF,IELE,TX)}

\text{C} \hspace{1cm} \text{*******************************************************}

\text{DIMENSION TEMPNI(10,1), TEMPNF(10,1), TX(1)}

\text{DIMENSION X(8)}

\text{DO 10 J=1, 8}

\hspace{1cm} \text{X(J) = TEMPNI(IELE,J)}

\text{10 CONTINUE}

\hspace{1cm} \text{TEMPI = XINTER(X,TX(1),TX(2),TX(3))}

\text{DO 20 J=1, 8}
\[ X(J) = \text{TEMPNF}(\text{IELE}, J) \]

20 CONTINUE

\[ \text{TEMPF} = \text{XINTER}(X, TX(1), TX(2), TX(3)) \]

\[ \text{TEMPER} = \text{TEMPF} - \text{TEMPI} \]

RETURN

END

C

FUNCTION XINTER(X,R,S,T)

C

DIMENSION X(1)

\[
\begin{align*}
\text{XINTER} &= (1/8.)*(1+R)*(1+S)*(1+T)*X(1) + (1-R)*(1+S)*(1+T)*X(2) \\
1 &+ (1-R)*(1-S)*(1+T)*X(3) + (1+R)*(1-S)*(1+T)*X(4) \\
2 &+ (1+R)*(1+S)*(1-T)*X(5) + (1-R)*(1+S)*(1-T)*X(6) \\
3 &+ (1-R)*(1-S)*(1-T)*X(7) + (1+R)*(1-S)*(1-T)*X(8))
\end{align*}
\]

RETURN

END
C.2 SUBROUTINE GTTH

C

******************************************************************************

SUBROUTINE GTTH(XC,NDD,NOD,COR,CONN,NUME,
1 NUMNP,E,V,ALPHA,TEMPNI,TEMPNF,TTH)

C

******************************************************************************

C THIS IS THE MAIN DRIVER OF THE PACKAGE. IT ALSO
C ASSEMBLES THE THE GLOBAL TTH VECTOR (TTH) FROM
C THE LOCAL ONES (LTTH)

COMMON /ABC/ AA, BB, CC, IELE
COMMON /ORIGIN/ XOR, YOR, ZOR

DIMENSION XC(2,1), NOD(10,1), COR(100,1), CONN(2,3,1)
DIMENSION TEMPNI(10,8), TEMPNF(10,8), TTH(1)
DIMENSION ETHERM(6), LTTH(3), C(6,6), TX(3), Q(3,3)
DIMENSION E(1), V(1), ALPHA(1)
INTEGER ORDER
REAL NTEMP, LTTH

DO 500 NODE=1, NDD
    AA=XC(1,NODE)*E1X+XC(2,NODE)*E2X+XOR
    BB=XC(1,NODE)*E1Y+XC(2,NODE)*E2Y+YOR
    CC=XC(1,NODE)*E1Z+XC(2,NODE)*E2Z+ZOR

50
CALL LOCEM3(TX, NOD, COR, CONN, NUME)

ORDER = (IELE-1)*3

TEMP = TEMPER(NUME, TEMPNI, TEMPNF, IELE, TX)
CALL STRAIN(ALPHA(IELE), TEMP, ETHERM)
CALL MTRL(E(IELE), V(IELE), C)
CALL TH(C, ETHERM, LTTH)
CALL TRANS(Q)

DO 50 I=1, 3
   DO 40 J=1,3
      TTH(ORDER+I) = TTH(ORDER+I) + Q(I,J)*LTTH(J)
   40    CONTINUE
50    CONTINUE
500   CONTINUE

END
C THIS SUBROUTINE CALCULATES THE LOCAL VECTOR CONTRIBUTIONS (LTTH)


DIMENSION C(6,1), ETHERM(1), LTTH(1)
DIMENSION NU(3,6), TMP(3,6)

REAL NU, LTTH

C INITIALIZING VARIABLES LOCAL TO THE SUBROUTINE

DO 50 I=1, 3
   LTTH(I) = 0.
   DO 40 J=1, 6
      TMP(I,J) = 0.
40    CONTINUE
50    CONTINUE

C ASSIGNING VALUES TO THE NU MATRIX

NU(1,1) = E3X
NU(1,2) = 0.
NU(1,3) = 0.
NU(1,4) = E3Y
NU(1,5) = 0.
NU(1,6) = E3Z

NU(2,1) = 0.
NU(2,2) = E3Y
NU(2,3) = 0.
NU(2,4) = E3X
NU(2,5) = E3Z
NU(2,6) = 0.

NU(3,1) = 0.
NU(3,2) = 0.
NU(3,3) = E3Z
NU(3,4) = 0.
NU(3,5) = E3Y
NU(3,6) = E3X

C EVALUATE THE LTTH MATRIX

DO 130 I=1, 6
  DO 120 J=1, 3
    DO 110 K=1, 6
      TMP(J,I) = TMP(J,I) + NU(J,K)*C(K,I)
 110    CONTINUE
120    CONTINUE
130    CONTINUE
DO 180 I=1, 3
DO 170 J=1, 6
    LTTH(I) = LTTH(I) + TMP(I,J)*ETHERM(J)
170    CONTINUE
    LTTH(I) = LTTH(I)*(-1.)
180    CONTINUE

END

C   ******************************************************************************
FUNCTION TEMPER(NUME,TEMPNI,TEMPNF,IELE,TX)
C   ******************************************************************************
C  GIVEN THE LOCATION OF POINT IN QUESTION (R,S,T
C  COORDINATES (TX VECTOR) AND THE ELEMENT
C  NUMBER IT IS LOCATED IN (IELE), THIS SUBROUTINE
C  CALCULATES ITS TEMPERATURE CHANGë FROM
C  ELEMENT TEMPERATURE CHANGE (IF TEMPFL=0.) OR
C  INTERPOLATES IT FROM THE NODAL INITIAL AND
C  FINAL TEMPERATURES (IF TEMPFL <>0)

DIMENSION TEMPNI(10,1), TEMPNF(10,1), TX(1)
DIMENSION X(8)

DO 10 J=1, 8
    X(J) = TEMPNI(IELE,J)
10    CONTINUE
TEMP1 = XINTER(X,TX(1),TX(2),TX(3))

DO 20 J=1, 8
    X(J) = TEMPNF(IELE,J)

20 CONTINUE

TEMPF = XINTER(X,TX(1),TX(2),TX(3))

TEMPER = TEMPF - TEMPI

RETURN

END

C

FUNCTION XINTER(X,R,S,T)

C

DIMENSION X(1)

XINTER= (1./8.)*((1+R)*(1+S)*(1+T)*X(1) + (1-R)*(1+S)*(1+T)*X(2)
  + (1-R)*(1-S)*(1+T)*X(3) + (1+R)*(1-S)*(1+T)*X(4)
  + (1+R)*(1+S)*(1-T)*X(5) + (1-R)*(1+S)*(1-T)*X(6)
  + (1-R)*(1-S)*(1-T)*X(7) + (1+R)*(1-S)*(1-T)*X(8))
RETURN
END

C *****************************************************************************
SUBROUTINE STRAIN(ALPHA, TEMP, ETHERM)
C *****************************************************************************

C THIS SUBROUTINE CALCULATES THE STRAIN DUE TO THERMAL STRESSES

DIMENSION ETHERM(1)

ETHERM(1) = ALPHA*TEMP
ETHERM(2) = ALPHA*TEMP
ETHERM(3) = ALPHA*TEMP
ETHERM(4) = 0.
ETHERM(5) = 0.
ETHERM(6) = 0.

RETURN
END
SUBROUTINE MTRI(E,V,C)

C THIS SUBROUTINE ASSEMBLES THE MATERIAL MATRIX
C (C) FROM GIVEN VALUES OF THE YOUNG'S MODULUS
C AND POISSON'S RATIO

DIMENSION C(6,1)

REL = E*(1-V)/( (1+V)*(1-2*V) )

C(1,1) = REL
C(1,2) = REL*V/(1-V)
C(1,3) = REL*V/(1-V)
C(1,4) = 0.
C(1,5) = 0.
C(1,6) = 0.
C(2,1) = REL*V/(1-V)
C(2,2) = REL
C(2,3) = REL*V/(1-V)
C(2,4) = 0.
C(2,5) = 0.
C(2,6) = 0.
C(3,1) = REL*V/(1-V)
C(3,2) = REL*V/(1-V)
C(3,3) = REL
C(3,4) = 0.
C(3,5) = 0.
C(3,6) = 0.
C(4,1) = 0.
C(4,2) = 0.
C(4,3) = 0.
C(4,4) = REL*(1-2*V)/(2*(1-V))
C(4,5) = 0.
C(4,6) = 0.
C(5,1) = 0.
C(5,2) = 0.
C(5,3) = 0.
C(5,4) = 0.
C(5,5) = REL*(1-2*V)/(2*(1-V))
C(5,6) = 0.
C(6,1) = 0.
C(6,2) = 0.
C(6,3) = 0.
C(6,4) = 0.
C(6,5) = 0.
C(6,6) = REL*(1-2*V)/(2*(1-V))
RETURN
END
C ***************************************************************

SUBROUTINE TRANS(Q)
C ***************************************************************

C THIS SUBROUTINE DEFINES THE Q MATRIX THAT IS USED TO TRANSFER TTH FROM GLOBAL TO LOCAL COORDINATES


DIMENSION Q(3,1)

Q(1,1) = E1X
Q(1,2) = E1Y
Q(1,3) = E1Z

Q(2,1) = E2X
Q(2,2) = E2Y
Q(2,3) = E2Z

Q(3,1) = E3X
Q(3,2) = E3Y
Q(3,3) = E3Z

END
Appendix D  Flow of Operations in the Code

D.1 SUBROUTINE GRTH

I) Determine the Gaussian integration order (INTPT), points (r, s, t), and weights (w).

II) Loop over elements of the finite element model.

A) Loop over the integration points for element at hand.

Symbolically, this is equivalent to

\[ \sum_{i=1}^{\text{INTPT}} \sum_{j=1}^{\text{INTPT}} \sum_{k=1}^{\text{INTPT}} f(r_i, s_j, t_k) w_i w_j w_k \]

1) Initialize variables.

2) Determine nodal coordinates of element at hand.

3) Calculate components of the Jacobian matrix [J].

4) Calculate components of [J]^{-1}.

5) Calculate components of the matrix of partial differentials of the shape functions with respect to the element local coordinates [DH].

6) Calculate components of [DDH]

\[ ([DDH] = [J]^{-1} [DH]) \]
7) Calculate strain-displacement matrix, \([B]\), from \([DDH]\).

8) Determine \([B]^T\).

9) Interpolate temperature change of node at hand from given nodal temperatures.

10) Calculate the thermal strain due to the temperature change.

11) Calculate the material matrix, \([C]\)

12) Calculate components of the resulting thermal loading correction vector. This is equivalent to \([R^th]\) of equation 2.4.11 of the text.

B) Sum the thermal loadings on all nodes of the element at hand.

D.2 SUBROUTINE GTTH

I) Loop over the nodes of crack elements.

A) Calculate global coordinates of the node at hand.

B) Locate the number of the finite element that contains it and its location in local element coordinates within the element. This operation utilizes SUBROUTINE LOCEM3 located in the SIFEH code.
C) Interpolate the temperature change of the node from given nodal temperatures.

D) Calculate the thermal strain due to the temperature change.

E) Calculate the material matrix.

F) Calculate the components of \( T^{th} \) using equation 2.5.5

G) Map \( T^{th} \) to local coordinates.

H) Assemble the \( T^{th} \) components for the node in the corresponding global vector.
Appendix E  Important Variables in the Code

E.1  SUBROUTINE GRTH

COR(NUMNP,8): array of nodal coordinates

NUME: number of elements in the finite element model

NOD(NUME,8): array of connectivities

E(NUME): array of Young's moduli for the different elements

V(NUME): array of Poisson's ratios for the different elements

ALPHA(NUME): array of coefficients of thermal expansion for the different elements

TEMPNI(NUME,8): array of initial nodal temperatures

TEMPNF(NUME,8): array of final nodal temperatures

RTH(NUMNP): vector of calculates thermal loads. This is \( R_{th} \) in the text.

D(3,3): the inverse of the Jacobian matrix which is the matrix of the partial differentials of the displacement interpolation functions with respect to the local element coordinates. Symbolically, the matrix is
\[ [D] = [J]^{-1} = \begin{bmatrix}
\frac{\partial x}{\partial r} & \frac{\partial y}{\partial r} & \frac{\partial z}{\partial r} \\
\frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} & \frac{\partial z}{\partial s} \\
\frac{\partial x}{\partial t} & \frac{\partial y}{\partial t} & \frac{\partial z}{\partial t}
\end{bmatrix}^{-1} \]

**DH(3,8):** matrix of the partial differentials of the shape functions with respect to the local coordinates.

Symbolically, this is

\[
[DH] = \begin{bmatrix}
\frac{\partial h_1}{\partial r} & \frac{\partial h_2}{\partial r} & \frac{\partial h_3}{\partial r} & \cdots & \frac{\partial h_8}{\partial r} \\
\frac{\partial h_1}{\partial s} & \frac{\partial h_2}{\partial s} & \frac{\partial h_3}{\partial s} & \cdots & \frac{\partial h_8}{\partial s} \\
\frac{\partial h_1}{\partial t} & \frac{\partial h_2}{\partial t} & \frac{\partial h_3}{\partial t} & \cdots & \frac{\partial h_8}{\partial t}
\end{bmatrix}
\]

**DDH(3,8):** matrix of the partial differentials of the shape functions with respect to the global coordinates,

\[ [DDH] = [D][DH]. \]

Symbolically, this matrix is

\[
[DDH] = \begin{bmatrix}
\frac{\partial h_1}{\partial x} & \frac{\partial h_2}{\partial x} & \frac{\partial h_3}{\partial x} & \cdots & \frac{\partial h_8}{\partial x} \\
\frac{\partial h_1}{\partial y} & \frac{\partial h_2}{\partial y} & \frac{\partial h_3}{\partial y} & \cdots & \frac{\partial h_8}{\partial y} \\
\frac{\partial h_1}{\partial z} & \frac{\partial h_2}{\partial z} & \frac{\partial h_3}{\partial z} & \cdots & \frac{\partial h_8}{\partial z}
\end{bmatrix}
\]

**B(6,24):** strain-displacement matrix. Its composition is detailed in Appendix A.
BB(24,6): transpose of [B], [B]T.

C(6,6): material matrix. Its composition is detailed in Appendix A.

ETHERM(6): vector of thermal strains for a given element. Its composition is detailed in Appendix A.

TMP(24,6): matrix for storing temporary multiplication results.

PRD(24): vector of temporary multiplication results.

LRTH(24): vector for storing temporary components of (Rth) for given element

X(8),Y(8),Z(8): global nodal coordinates of element at hand

R(3),S(3),T(3): location of Gaussian integration points.

W(3): Gaussian integration weights.

INTPT: Gaussian integration order.

DET: the Jacobian, J, which is the determinant of [J].
E.2 SUBROUTINE GTTH

XC(2, NDD): matrix of nodal coordinates of crack elements with respect to the local coordinate system of the crack.

NDD: number of nodes on the crack element.

NOD: same as that in SUBROUTINE GRTH.

COR: same as that in SUBROUTINE GRTH.

CONN(2, 3, NUME): matrix of the ranges of the finite element nodal coordinates from minimum to maximum in all three global directions.

NUME: same as that in SUBROUTINE GRTH.

E, V, ALPHA: same as that in SUBROUTINE GRTH.

TEMPNI, TEMPNF: same as that in SUBROUTINE GRTH.

TTH(NDD*3): calculated vector of tractions on the crack surface due to the thermal conditions. This is equivalent to \( T^{th} \) in the text.

AA, BB, CC: global coordinates of the crack element at hand.

IELE: number of the finite element that the crack node is located in.
E1X,E1Y,E1Z:    global components of the orthogonal triad of unit
E2X,E2Y,E2Z    vectors formed by E1, E2, and E3, where E1 and E2
E3X,E3Y,E3Z    lie in the plane of the fracture.

XOR,YOR,ZOR:    global coordinates of the origin of the coordinate
                system which is local to the crack.

LTTH(3):        \( \{T^\text{th}\} \) vector of crack node at hand.

Q(3,3):         rotation matrix to map the calculates \( \{T^\text{th}\} \) from
                global to local coordinates. This corresponds to \([Q]\)
                in the text.
References


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SUBJECT TO THERMAL LOADING

by

RIAD JOSEPH BSAIBES

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